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Kink-antikink collisions in sine-Gordon and ϕ^4 models: Problems in the variational approach

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In this paper, a collective-coordinate description of a breatherlike solution of the perturbed sine-Gordon equation is considered. It is shown both numerically and analytically that the equations describing the evolution of the breather parameters are ill defined. This feature is shown to arise because the equations are obtained through a projection on a null vector. It is shown to be present also in collective-coordinate descriptions of the kink-antikink collision in the ϕ^4 model. Alternative *Ansätze* that do not cause singularities are presented.

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I. INTRODUCTION

There are many mathematical techniques that can be used to obtain the analytic solution in an integrable system. The solutions are characterized by a number of constant parameters that come naturally as action variables from the inverse scattering method [1]. This is not possible when the system is perturbed. One idea is to assume that the solution depends only on a small number of time-dependent parameters (collective coordinates) which have a physical meaning. The choice of the collective coordinates is arbitrary even though one is led to them by introducing time dependence into the constant parameters of the unperturbed system. By this method one hopes to reproduce the important features in the time evolution of nonlinear waves. A significant reduction in the number of degrees of freedom is achieved by going from the nonlinear partial differential equation (PDE) to a set of ordinary differential equations (ODE's). However introducing many modes can lead to a competition between the chosen collective coordinates. In particular some coordinates can be redundant. It may also happen that the particular form of the *Ansatz* can lead to ill-defined equations as will be shown in the present work.

For the sine-Gordon and ϕ^4 equations many efforts have been applied to get a simplified description of the dynamics. The use of a single collective coordinate describing the kink position in the sine-Gordon equation is very restrictive. The addition of a time-dependent kink width by Rice and Mele [2] in the study of lightly doped polyacetylene better describes the deformable particle character of the kink motion. Such an object called a "wobbling kink" was shown to exist by Segur both for sine-Gordon and ϕ^4 [3] models even in the absence of perturbations. To demonstrate this he used asymptotic expansions. Its stability, however, could not be proved for the ϕ^4 model while some qualitative arguments by Campbell [3] make it questionable for the sine-Gordon model. The collective-coordinate description has also been successful in describing the evolution of a sine-Gordon kink submitted to a spatial perturbation in order to model a nonuniform Josephson junction with a variable maximum Josephson current [4]. This inhomogeneity creates a local potential for the fluxon which can compete with the driving frequency and lead to chaos via period-doubling bifurcations. The remarkable agreement between the dynamics of the perturbed PDE and the ODE's for the set of two collective coordinates [4] showed that this particular choice of collective coordinates was a good one.

Many different sets of collective coordinates have been used by different authors for the ϕ^4 model in studying kink-antikink collisions where interesting resonance phenomena appear due to the interchange of energy through internal oscillations [5]. In fact, these were specifically taken into account as extra degrees of freedom by Sugiyama [6]. Even though he did not take into account the width coordinate a deformation of the kink-antikink was possible through the internal modes. Jeyadev and Schrieffer [7] extended this by using a relativistic covariant *Ansatz* but in order to make the calculations tractable they did not take the phonon contribution to be covariant. The phonon coordinate blew up during the collision. It will be shown that it would not have blown up if the phonon contribution was taken to be fully covariant. Campbell, Schonfeld, and Wingate [8] introduced a simple *Ansatz* with a translational and a shape degree of freedom to calculate the interaction between two kinks. A detailed numerical analysis of the equations by Flesch [9] showed that the shape mode blew up during the collision. For the sine-Gordon equation, Legrand guided by an algebraic identity gave a two-collective-coordinate *Ansatz* which he used for the study of a perturbed breather [10]. There is a sign error in the Lagrangian of [10] which when corrected introduces a mathematical singularity that cannot be removed. The shape mode coordinate blows up when the breather is "flat." In this paper all these "singular behaviors" will be explained. The reason is that the Lagrange equations are obtained through a projection on a vector that becomes zero at one point in the evolution.

The paper is organized as follows. In Sec. II, the variational procedure and the equations of motion are presented. Section III shows evidence for the singular character of the equations by means of two accurate numerical schemes. Section IV explains this feature for the sine-Gordon collective-coordinate problem and for a ϕ^4 collective-coordinate study. In Sec. V a possible way of eliminating this ill definition is presented and some *Ansätze* are introduced. Concluding remarks are given in Sec. VI.

II. VARIATIONAL APPROACH

Consider the perturbed sine-Gordon equation:

$$\phi_{tt}-\phi_{xx}+\sin\phi=F(\phi,\phi_t,t)\ . \quad (1)$$

When $F=0$, Eq. (1) can be integrated exactly and two well-known solutions are [1] the breather

$$\phi_B(x,t)=4\arctan\left[\frac{k_B\sin(\omega_B t+\phi_B)}{\omega_B\cosh(k_B x)}\right], \quad (2)$$

where $k_B^2=1-\omega_B^2$ and the kink-antikink

$$\phi_{K\bar{K}}(x,t)=4\arctan\left[\frac{\sinh(\gamma_L ut)}{u\cosh(\gamma_L x)}\right], \quad (3)$$

where $\gamma_L=1/\sqrt{1-u^2}$ is the Lorenz factor. Formulas (2) and (3) can be seen as special cases of

$$\phi(x,y(t),k(t))=4\arctan\left[\frac{\sinh[y(t)]}{\cosh[k(t)x]}\right], \quad (4)$$

where $y(t)$ and $k(t)$ have different expressions depending on whether the solution is a kink-antikink or a breather. This *Ansatz* relies on an algebraic identity between the sum of a soliton and antisoliton profiles and the expression on the right-hand side (rhs) of (4) minus 2π. It was put forth by Legrand [10]. The collective-coordinate approach is to assume that the solution can be written as in Eq. (4) when the perturbation is present. It order to derive the evolution equations for y and k, one could insert (4) into (1) but there would still by an x dependence. Instead, a variational approach is used. Equation (1) with $F=0$ can be derived from the following Lagrangian density:

$$l=\tfrac{1}{2}\phi_t^2-\tfrac{1}{2}\phi_x^2-(1-\cos\phi) \quad (5)$$

by writing that the variation of $\int\int l\,dx\,dt$ is zero. Assuming that the solution can be written as in Eq. (4), the evolution of y and k is then obtained from the usual Lagrange equations derived from the Lagrangian $L(y,\dot{y},k,\dot{k},t)=\int l\,dx$ where expression (4) for ϕ is used to compute (5). The terms in the perturbation that cannot be incorporated in the Lagrangian density such as the damping are treated separately [10]. If

$$F=\epsilon\sin\omega t-\delta\phi_t \quad (6)$$

the equations of motion are

$$P=\frac{\partial L}{\partial\dot{y}}\ , \quad (7a)$$

$$Q=\frac{\partial L}{\partial\dot{k}}\ , \quad (7b)$$

$$\frac{dP}{dt}+\delta P=\frac{\partial L}{\partial y}\ , \quad (7c)$$

$$\frac{dQ}{dt}+\delta Q=\frac{\partial L}{\partial k}\ , \quad (7d)$$

where

$$\begin{aligned}L=&\ \dot{y}^2\frac{8}{k}\left[1+\frac{2y}{\sinh 2y}\right]-\dot{y}\dot{k}16\frac{y}{k^2}\\&+\dot{k}^2\frac{2}{3k^3}\left[(\pi^2+4y^2)\left[1-\frac{2y}{\sinh 2y}\right]+8y^2\right]\\&-8k\left[1-\frac{2y}{\sinh 2y}\right]-\frac{8}{k}(\tanh y)^2\left[1+\frac{2y}{\sinh 2y}\right]\\&+4\pi\frac{y}{k}\epsilon\sin\omega t\end{aligned} \quad (7e)$$

is the Lagrangian and $P(Q)$ is the momentum associated to y (k), respectively. In the original paper of Legrand, a sign error was made in the coefficient of the $\dot{k}^2$ term in L. It was written to be $(\pi^2+4y^2)[1+(2y/\sinh 2y)]+8y^2$. We will see that this mistake completely hid the real behavior of the solution around $y=0$. All the terms in L except for the coefficient of $\dot{y}^2$ become zero when $y=0$ so that the k oscillator becomes uncoupled from the y oscillator and its mass goes to zero. The frequency of the k mode is then expected to go to infinity leading to numerical problems when y is small.

III. NUMERICAL EVIDENCE FOR A SINGULAR SOLUTION

The standard way to integrate the two second-order ODE's (7) is to transform them into a system of first-order differential equations using as variables (y,k,P,Q). The evolution of P and Q is given by (7c) and (7d) while the evolution of y and k is obtained by inverting the system obtained from (7a) and (7b):

$$\begin{bmatrix}P\\Q\end{bmatrix}=\begin{bmatrix}16\dfrac{\alpha}{k} & -16\dfrac{y}{k^2}\\ -16\dfrac{y}{k^2} & \dfrac{4}{3k^3}[\gamma(2-\alpha)+8y^2]\end{bmatrix}\begin{bmatrix}\dot{y}\\\dot{k}\end{bmatrix},$$
$$\alpha=1+\frac{2y}{\sinh 2y}\ ,\quad \gamma=\pi^2+4y^2\ . \quad (8)$$

The value $y=0$ makes the right-hand side matrix of (8) noninvertible indicating again numerical problems, even in the absence of perturbations. The numerical study has been done setting the perturbation terms to zero to see if the *Ansatz* captures the unperturbed dynamics where the exact solution is known. All the numerical methods that were used failed to integrate (7) and match the pure breather analytic solution of (1) when $F=0$. Even though the results are negative they yield some insight into the problem. Three main methods have been used: ODE integrators, matching techniques, and an energy conserving integration scheme.

A standard fixed step fourth-order Runge-Kutta method gives a jump in relative error in the pure breather case as y crosses zero and fails to conserve energy. A variable step method [11] allows us to approach $y=0$ up to 10^{-3} with $\dot{k}$ being of the order of 10^{-10} for the unperturbed problem where the exact solution is $\dot{k}=0$. The singularity could be avoided by an expansion for small y that eliminates the terms in the kinetic energy of the k oscillator whose mass vanishes. This leads to a first-order equation for k which makes $\dot{k}$ discontinuous. The lack of symmetry of the solution around $y=0$ does not allow any matching to be done that would permit the y variable to cross 0. The ill definition of the equation for the k collective coordinate also appears when looking at small perturbations $\tilde{y}$ and $\tilde{k}$ around a breather near the instant when $y\approx 0$, i.e., when the breather is almost flat. The linearized equations are

$$\ddot{\tilde{y}}+\tilde{y}=0 , \tag{9a}$$

$$\dot{\tilde{k}}=0 \tag{9b}$$

so that $\tilde{y}$ is oscillatory but $\tilde{k}$ has to remain constant. On the contrary for a kink both the modulations of the position y and width k can have an oscillatory behavior. For the breather problem, assuming that the strict conservation of energy could prevent the singularity, a discrete energy conserving integration scheme suggested by Vazquez [12] was implemented. It is a finite difference discretization of the Lagrange equations. The exact expressions can be found in [12]. A discrete equivalent of the energy

$$E=P\dot{y}+Q\dot{k}-L \tag{10}$$

can be defined and the work equation obtained from (7),

$$\frac{dE}{dt}=-\delta(\dot{y}P+\dot{k}Q)-\frac{dL}{dt} , \tag{11}$$

can be written in a discrete form so that the scheme is conservative in the absence of damping. At each step a second-degree equation has to be solved for $\dot{y}$ and $\dot{k}$ making the scheme implicit. There is still a problem when y approaches zero because the roots of the second-degree equation for $\dot{k}$ become complex. For $y\approx 0$ the numerical scheme has no solution. In fact energy considerations for the continuous equations (7) indicate a blowup of $\dot{k}$ when $y=0$.

Consider the Hamiltonian associated to Eqs. (7) in the absence of damping or forcing:

$$H=8\frac{\dot{y}^2\alpha}{k}-16y\frac{\dot{y}\dot{k}}{k^2}+2\frac{\dot{k}^2}{k^3}[\gamma(2-\alpha)+8y^2] +8k(2-\alpha)+\frac{8}{k}(\tanh y)^2\alpha . \tag{12}$$

Solving (12) for $\dot{k}$ and taking y small, we have

$$\dot{k}=\frac{\frac{8\dot{y}}{k^2y}+\left[\left(\frac{8\dot{y}}{k^2y}\right)^2-\frac{1}{y^2}\frac{2}{k^3}\left(\frac{2\pi^2}{3}+8\right)\left(\frac{16\dot{y}^2}{k}-H\right)+O(y^2)\right]^{1/2}}{\left(\frac{2}{k^3}\right)\left(\frac{2\pi^2}{3}+8\right)+O(y^2)} . \tag{13}$$

This shows that $\dot{k}$ is infinite for $y=0$ unless $(16\dot{y}^2/k)-H=0$. In that case one of the values is infinite while the other is zero; the latter being associated to the pure breather or the pure kink-antikink solution. From these numerical results one expects that the singularity in the solutions for $y=0$ is due to the form of the collective-coordinate equations themselves and not to any numerical scheme used for the integration. It turns out that one can predict it from the solution *Ansatz* (4).

IV. ANALYTICAL ARGUMENTS EXPLAINING THE SINGULARITY

The Lagrange equations derived from

$$L(y,\dot{y},k,\dot{k},t)=\int l(\phi_t,\phi_x,\phi,t)dx \tag{14}$$

have a solution that is undetermined when $y=0$. Legrand [10] examined in detail the procedure in which (4) is substituted into (14). The spatiotemporal dependence of ϕ in (4) can be written as $\phi=\phi(x,a_i(t))$ where the a_i are the collective coordinates. The Lagrange equations from (14),

$$\frac{\partial L}{\partial a_i}-\frac{d}{dt}\left[\frac{\partial L}{\partial \dot{a}_i}\right]=0 , \tag{15}$$

imply

$$\int_{-\infty}^{+\infty}dx\left[\frac{\partial l}{\partial\phi}\frac{\partial\phi}{\partial a_i}+\frac{\partial l}{\partial\phi_x}\frac{\partial\phi_x}{\partial a_i} +\frac{\partial l}{\partial\phi_t}\frac{\partial\phi_t}{\partial a_i}-\frac{\partial}{\partial t}\left[\frac{\partial l}{\partial\phi_t}\frac{\partial\phi_t}{\partial\dot{a}_i}\right]\right]=0 . \tag{16}$$

Using the fact that $\partial\phi_t/\partial\dot{a}_i=\partial\phi/\partial a_i$, integrating by parts with respect to x, and assuming that $\partial\phi/\partial a_i$ vanishes at $\pm\infty$, the Lagrange equations (15) imply [10]

$$\int_{-\infty}^{+\infty} dx \left[\frac{\partial l}{\partial \phi} - \frac{\partial}{\partial t}\left[\frac{\partial l}{\partial \phi_t}\right] - \frac{\partial}{\partial x}\left[\frac{\partial l}{\partial \phi_x}\right]\right] \frac{\partial \phi}{\partial a_i} = 0 \ . \tag{17}$$

The expression in brackets is the left-hand side of the sine-Gordon equation as obtained from the condition that the spatiotemporal variation of l is stationary. Therefore (17) can be seen as a projection of the sine-Gordon operator onto the mode $\partial\phi/\partial a_i$. This situation does not change when the sine-Gordon equation is perturbed; the evolution equations are still given by (17). For our problem the coordinates $a_i(t)$ are the pair $(y(t),k(t))$ so that

$$\frac{\partial \phi}{\partial y} = 4\frac{\cosh(y)\cosh(kx)}{(\cosh kx)^2 + (\sinh y)^2} , \tag{18}$$

$$\frac{\partial \phi}{\partial k} = -4\frac{\sinh(y)\sinh(kx)x}{(\cosh kx)^2 + (\sinh y)^2} . \tag{19}$$

The first mode is nonzero for all values of y but the second mode is zero when $y=0$ (for all x) so that the Lagrange equation for the evolution of k is automatically satisfied no matter what the dependence is of k and x on time. For $y=0$, the projection is done on a zero mode, therefore giving no information. Note that this problem only occurs for a breather or kink-antikink *Ansatz* and not for a pure kink.

If one chooses an *Ansatz* for the solution like the one of Scott and McLaughlin [13] instead of the (y,k) coordinates the problem remains unchanged. Take for example the breather *Ansatz* of [13]:

$$\phi_B = 4\arctan\left[\frac{\tan(\nu)\sin(T)}{\cosh[x\sin(\nu)]}\right] . \tag{20}$$

When $T=0$, $\partial\phi_B/\partial\nu = 0$ so that again the projection is done on a null vector. This leads one to believe that it is the form of the *Ansatz* that causes the problem. In fact any *Ansatz* of the type

$$\phi(x,y(t),k(t)) = 4\arctan\left[\frac{f(y(t),k(t))}{g(y(t),k(t),x)}\right] , \tag{21}$$

where f can be zero, is doomed because the partial derivatives

$$\frac{\partial \phi}{\partial k} = \frac{4}{1+(f/g)^2}\left[\frac{f_k}{g} - \frac{f}{g^2}g_k\right] , \tag{22}$$

$$\frac{\partial \phi}{\partial y} = \frac{4}{1+(f/g)^2}\left[\frac{f_y}{g} - \frac{f}{g^2}g_y\right] \tag{23}$$

are proportional when $f=0$ because the terms f_y and f_k carry no x dependence, therefore leading as above to ill-defined evolution equations.

The ϕ^4 problem. The ϕ^4 model [1]

$$\phi_{tt} - \phi_{xx} - (\phi - \phi^3) = 0 \tag{24}$$

can be obtained from (1) by expanding the sine term in Taylor series and keeping only the two first terms of the expansion. Even though the equation is not integrable an exact solution is known—the kink (or antikink):

$$\phi(x,t) = \pm\tanh\left[\frac{1}{\sqrt{(2)}}\frac{(x-vt)}{\sqrt{1-v^2}} + \xi\right] , \tag{25}$$

where ξ is an arbitrary phase. To describe collisions between kinks for this model collective coordinates have been used. It particular Flesch [9] used an *Ansatz:*

$$\phi(x,x_0(t),y_0(t)) = 1 - \tanh\left[\frac{y_0(x-x_0)}{\sqrt{2}}\right] + \tanh\left[\frac{y_0(x+x_0)}{\sqrt{2}}\right] , \tag{26}$$

where x_0 is the center-of-mass variable and y_0 is the inverse of the width of the kinks. The Lagrangian he obtains is very similar to (7e) in the sense that when x_0 goes through 0 the coefficients of the terms in $\dot{y}_0^2$ and $\dot{x}_0\dot{y}_0$ go to zero. In fact

$$\phi_{y_0} = -\left[\operatorname{sech}\left[\frac{y_0(x-x_0)}{\sqrt{2}}\right]\right]^2 \frac{(x-x_0)}{\sqrt{2}} + \left[\operatorname{sech}\left[\frac{y_0(x+x_0)}{\sqrt{2}}\right]\right]^2 \frac{(x+x_0)}{\sqrt{2}} \tag{27}$$

is zero for $x_0=0$ so that again the projection is done on a null vector. The problem cannot be fixed by introducing $\dot{x}_0$ in the *Ansatz* or by adding a radiation term because the projection on the y_0 mode is the problem. Exactly as for the (y,k) variables, the numerical simulations show that $\dot{y}_0$ blows up when $x_0=0$. From the Hamiltonian Flesch shows [9] that $\dot{y}_0$ necessarily goes to ∞ when $x_0=0$ unless $\dot{x}_0$ is such that $\frac{1}{2}m_1\dot{x}_0^2 + V - H_0 = 0$ where V is the potential energy and H_0 the total energy. His numerics use the algebraic differential equation solver DASSL developed by Petzold [14]. Such an integrator uses the functional form for the differential equation $F(\Phi,\dot{\Phi},t)=0$ and minimizes F by computing the correct values of Φ and $\dot{\Phi}$. Even though it does a better job than all the routines mentioned above, because the "jump" in the value of the Hamiltonian is small at the crossing [9], it still cannot be used for a study of the long-time behavior of the perturbed sine-Gordon equation because the amplitude of the "jump" is likely to increase at every crossing.

Prior to the study of Flesch, Jeyadev and Schrieffer [7] had done a collective-coordinate study of the ϕ^4 model using an *Ansatz* derived from the Lorenz covariant solution of the linearized ϕ^4 equation around a static kink. The complete *Ansatz* was

$$\phi(\alpha(t),\dot{\alpha}(t)A(t),B_Q(t),xt) = 1+\tanh y_- - \tanh y_+ + A(t)\left[\phi_1(-)\cos\frac{F_1(t-\dot{\alpha}x)}{\sqrt{1-\dot{\alpha}^2}} - \phi_1(+)\cos\frac{F_1(t+\dot{\alpha}x)}{\sqrt{1-\dot{\alpha}^2}}\right] + \sum_Q B_Q(t)\left[\phi_Q(-)\cos\frac{F_Q(t-\dot{\alpha}x)}{\sqrt{1-\dot{\alpha}^2}} - \phi_Q(+)\cos\frac{F_Q(t+\dot{\alpha}x)}{\sqrt{1-\dot{\alpha}^2}}\right], \tag{28a}$$

where

$$y_\pm = \frac{x\pm\alpha}{\sqrt{2}\sqrt{1-\dot{\alpha}^2}}, \tag{28b}$$

2α is the separation between the kink and antikink, ϕ_1 is the "shape" mode associated with its frequency F_1,

$$\phi_1(\pm) = \tan(y_\pm)\text{sech}(y_\pm), \tag{28c}$$

and ϕ_Q are the phonon modes associated with their frequency F_Q. The calculations of the Lagrangian were intractable with expression (28) so the authors of [7] used a reduced *Ansatz* neglecting the $\dot{\alpha}$ term in $y_\pm$:

$$\phi(\alpha(t),A(t),x,t) = 1+\tanh y_- - \tanh y_+ + A(t)[\phi_1(-)-\phi_1(+)]. \tag{29}$$

The A coordinate blew up during the collision as could be expected from the fact that $\phi_A=0$ when $\alpha=0$. The full *Ansatz* is such that ϕ_A is nonzero when $\alpha=0$ because the $\dot{\alpha}$ dependence is different in the two terms. Keeping the full *Ansatz* (28) cannot be done in practice because of the complication of the integrals involved in evaluating the Lagrangian. In the following section simpler *Ansätze* are presented that do not cause ill-defined evolution equations.

V. ALTERNATIVE *ANSÄTZE* FOR SINE-GORDON AND ϕ^4 MODELS

Because the ill definition of the equations is due to the fact that the Lagrange equations are obtained by a projection on a null vector, a way to fix things is not to do a simple projection anymore. Introducing an $\dot{a}_i$ dependency in the *Ansatz* leads to a Lagrangian $L(a_i,\dot{a}_i,\ddot{a}_i)$. The Lagrange equation for a_i is now

$$\frac{\partial L}{\partial a_i} - \frac{d}{dt}\left[\frac{\partial L}{\partial \dot{a}_i}\right] + \frac{d^2}{dt^2}\left[\frac{\partial L}{\partial \ddot{a}_i}\right] = 0. \tag{30}$$

It implies

$$\int_{-\infty}^{+\infty} dx\left[\left[\frac{\partial l}{\partial\phi}\frac{\partial\phi}{\partial a_i} + \frac{\partial l}{\partial\phi_x}\frac{\partial\phi_x}{\partial a_i} + \frac{\partial l}{\partial\phi_t}\frac{\partial\phi_t}{\partial a_i}\right] - \frac{\partial}{\partial t}\left[\frac{\partial l}{\partial\phi}\frac{\partial\phi}{\partial\dot{a}_i} + \frac{\partial l}{\partial\phi_x}\frac{\partial\phi_x}{\partial\dot{a}_i} + \frac{\partial l}{\partial\phi_t}\frac{\partial\phi_t}{\partial\dot{a}_i}\right] + \frac{\partial^2}{\partial t^2}\left[\frac{\partial l}{\partial\phi_t}\frac{\partial\phi_t}{\partial\ddot{a}_i}\right]\right] = 0. \tag{31}$$

It can be noticed that $\partial\phi_t/\partial\ddot{a}_i = \partial\phi/\partial\dot{a}_i$. By integrating by parts with respect to x and assuming that $(\partial l/\partial\phi_x)(\partial\phi/\partial a_i)$ and $\partial/\partial t[(\partial l/\partial\phi_x)(\partial\phi/\partial\dot{a}_i)]$ tend to zero at $\pm\infty$, Eq. (31) is equivalent to

$$\int_{-\infty}^{+\infty} dx\left\{\left[\left[\frac{\partial l}{\partial\phi} - \frac{\partial}{\partial x}\left[\frac{\partial l}{\partial\phi_x}\right]\right]\frac{\partial\phi}{\partial a_i}\right] - \frac{\partial}{\partial t}\left\{\left[\frac{\partial l}{\partial\phi} - \frac{\partial}{\partial x}\left[\frac{\partial l}{\partial\phi_x}\right]\right]\frac{\partial\phi}{\partial\dot{a}_i}\right]\right\} + \frac{\partial l}{\partial\phi_t}\frac{\partial\phi_t}{\partial a_i} - \frac{\partial}{\partial t}\left[\frac{\partial l}{\partial\phi_t}\frac{\partial\phi_t}{\partial\dot{a}_i}\right] + \frac{\partial}{\partial t}\left[\frac{\partial}{\partial t}\left[\frac{\partial l}{\partial\phi_t}\frac{\partial\phi}{\partial\dot{a}_i}\right]\right]\Bigg] = 0. \tag{32}$$

Now use the fact that

$$\frac{\partial\phi_t}{\partial a_i} = \frac{\partial}{\partial t}\left[\frac{\partial\phi}{\partial a_i}\right]$$

and write

$$\frac{\partial l}{\partial\phi_t}\frac{\partial\phi_t}{\partial a_i} = \frac{\partial}{\partial t}\left[\frac{\partial l}{\partial\phi_t}\frac{\partial\phi}{\partial a_i}\right] - \frac{\partial}{\partial t}\left[\frac{\partial l}{\partial\phi_t}\right]\frac{\partial\phi}{\partial a_i}$$

so that the whole expression becomes

$$\int_{-\infty}^{+\infty} dx\left[\Xi\frac{\partial\phi}{\partial a_i} - \frac{\partial}{\partial t}\left[\Xi\frac{\partial\phi}{\partial\dot{a}_i}\right] + \frac{\partial}{\partial t}\left\{\frac{\partial l}{\partial\phi_t}\left[\frac{\partial}{\partial t}\left[\frac{\partial\phi}{\partial\dot{a}_i}\right] - \frac{\partial\phi_t}{\partial\dot{a}_i} + \frac{\partial\phi}{\partial a_i}\right]\right\}\right] = 0, \tag{33a}$$

where

$$\Xi=\frac{\partial l}{\partial\phi}-\frac{\partial}{\partial t}\left[\frac{\partial l}{\partial\phi_t}\right]-\frac{\partial}{\partial x}\left[\frac{\partial l}{\partial\phi_x}\right]. \quad (33b)$$

The last term is identically zero so that the Lagrange equation is [7]

$$\int_{-\infty}^{+\infty}dx\left[\Xi\frac{\partial\phi}{\partial a_i}-\frac{\partial}{\partial t}\left[\Xi\frac{\partial\phi}{\partial\dot a_i}\right]\right]=0\ , \quad (34)$$

which is no longer a simple projection. Following this idea, a simple *Ansatz* that can be introduced for the breather problem is

$$\phi(x,y(t),k(t))=4\arctan\left[\frac{\sinh[y(1+\dot k)]}{\cosh kx}\right]. \quad (35)$$

While this *Ansatz* is arbitrary, it is very appropriate to make our point for the removal of the divergence in the equation for k. It is not also unreasonable since any shape oscillation can cause a small extension or contraction of the breather. When y is large the $\dot k$ term leads to a wobbling kink-antikink pair. The reason for setting y as a factor is to avoid a forced time dependence of k. In the absence of perturbations $\dot k=0$ so that the pure breather or kink-antikink solutions still exist. For all these reasons it is hoped that this *Ansatz* will lead to a successful quantitative comparison with the solution of the perturbed PDE. The evolution equations are currently being derived.

For the ϕ^4 problem, an *Ansatz* of the form

$$\phi(x,x_0(t),y_0(t))=1-\tanh\left[\frac{y_0[x-x_0(1+\dot y_0)]}{\sqrt{2}}\right]+\tanh\left[\frac{y_0[x+x_0(1+\dot y_0)]}{\sqrt{2}}\right] \quad (36)$$

eliminates the singularity for $x_0=0$. Again, it is not unreasonable to assume that the separation of the kink-antikink pair depends on the shape variable y_0. It is hoped using this *Ansatz* to obtain a quantitative agreement with the solution of the partial differential equation.

VI. DISCUSSION AND SUMMARY

The breather dynamics and its transition to a kink-antikink pair is an important source of chaos in the perturbed sine-Gordon equation. This has been shown by solving directly the partial differential equation that describes the time evolution of a field or many coupled oscillators in the discrete case that requires extensive computations. Such a direct approach does not elucidate the simplified low-dimensional mechanisms for the transition to chaos for the sine-Gordon equation or the complicated resonance structure for the unperturbed but nonintegrable ϕ^4 system. Several authors therefore used the collective-coordinate approach [6,7,9,10]. In all these cases the choice of the *Ansatz* introduced mathematical singularities. It has been shown in Sec. IV that the source of the singularity lies on the projection on a mode that vanishes at one instant in the evolution of the system. This was established by writing the Lagrange equations. At this point it should be remarked that the problem is attached to only one of the two coordinates. Introducing a relativistic effect on the problem-free coordinate will not remedy the situation. For example, in the (y,k) problem considered introducing $\dot y$ in the *Ansatz* is not useful because it is the effective mass connected with $\dot k^2$ in the Lagrangian that vanishes. Section V showed the essential mathematical ingredient that a new *Ansatz* must have. For the breather an arbitrary $\dot k$ dependence was introduced in the *Ansatz* leading to a Lagrangian containing a $\ddot k$ dependence and a fourth-order nonsingular evolution equation through a second-order variational equation. In the case of ϕ^4, a dependence of the kink-antikink separation was introduced. It is then clear that the evolution equation of the shape mode is not singular. The same goal could have been achieved by keeping the complete relativistic *Ansatz* introduced in [7]. This would have introduced very complicated integrals over x, the value of which could not have been calculated analytically.

The ill-defined character of the evolution equations for one of the collective coordinates can be found in other nonlinear problems like the double sine-Gordon equation written as [15]

$$\phi_{tt}-\phi_{xx}+(\tanh R_0)^2\sin\phi+2(\mathrm{sech} R_0)^2\sin\frac{\phi}{2}=0\ . \quad (37)$$

The equation is nonintegrable but a solution is known—the 4π kink:

$$\phi(x,R_0)=-4\arctan(e^{-x+R_0})+4\arctan(e^{x+R_0})=4\arctan\left[\frac{\sinh x}{\cosh R_0}\right] \quad (38)$$

so that collective-coordinate methods can be used. In [15], the following *Ansatz* was used

$$\phi(x,R(t))=4\arctan\left[\frac{\sinh x}{\cosh[R(t)]}\right] \quad (39)$$

in order to study the fluctuations of the separation R between the two kink components. It is clear that $\phi_R=0$ when $R=0$ leading to a vanishing mass in the Lagrangian. Fortunately, the parameter R never goes to zero because the interaction potential between the two kink components is minimum for $R>0$ as long as $R_0>0$. Therefore the ill-defined character of the equations is not apparent in the numerics.

Collective-coordinate methods do not have a range of validity like standard perturbation methods based on the theory of inverse scattering [13]. Therefore they remain empirical and should not be used to predict results of the numerical integration of the PDE. For example, Legrand [10] compares the results of a PDE simulation on a perturbed breather with the collective-coordinate evolution obtained from the solution *Ansatz* (4). Despite a sign error he finds good agreement. The reason for that is that there is very little interplay between the y and k variables except when y is close to zero. Elsewhere the $\dot{k}$ terms are very small. Computing $(y(t),k(t))$ with the wrong sign in (73) and a pure breather initial condition with $k=0.1$ leads to a value of $\dot{k}$ about 10^{-3}, clearly nonzero but still small. The only variable that plays a significant role is y. A detailed study of the behavior of the collective-coordinate ODE's would have pointed that out. In the same perspective but for the ϕ^4 model, Fei and Vazquez [16] took the Lagrangian obtained from the *Ansatz* (26) and eliminated the terms causing singularities when $x_0=0$. They justified this by the fact that these terms decay exponentially fast with x_0 and the claim that the *Ansatz* (26) is completely unrealistic when $x_0 \approx 0$. The equations they obtain do not mimic the dynamics of the PDE so the authors of [16] proceed to set to zero the interaction term between the shape mode and the position mode when $x_0<0$ and to rescale it by an arbitrary parameter λ for $x_0>0$. Despite these rather severe approximations Fei and Vazquez find a value of λ for which they observe a remarkable qualitative agreement with the extensive PDE simulations of [8]. It seems natural then to think that this resonance phenomena could be found in very simple approximations. The reason for our advocating a more complicated *Ansatz* is because of the hope of a quantitative agreement with the PDE so that one would be able to model completely the kink-antikink collisions without an adjustable parameter. With that idea in mind, the evolution equations are currently being derived and coded.

Recently it came to our attention that Boesch, Stancioff, and Willis [17] treated the problem of multiple collective variables of nonlinear Klein-Gordon equations. They use the Dirac treatment of constrained Hamiltonian systems. Their calculations are simplified by using a projection procedure that bears some similarities to the projection described in Eq. (17). They applied the procedure to the double sine-Gordon equation using an *Ansatz* for a 4π kink in the form

$$\phi=\sigma(y+R)-\sigma(R-y)+\chi \ , \tag{40}$$

where

$$\sigma(x)=4\arctan(e^x), \quad y=\gamma(x-X) \ .$$

γ is a parameter, $X(t)$ is the center of mass, $R(t)$ the separation of the two subkinks, and χ is the radiation field. They even considered a relativistically correct *Ansatz* with $\gamma=1/\sqrt{1-\dot{X}^2}$ so that the equation of motion includes d^4X/dt^4. This however does not eliminate the potential singularity we discussed earlier because $\partial\phi/\partial R=0$ when $X=0$.

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